$20 \times 13 \times 22$ cm. We are now working further in construction of a more compact and lightweight high valtage supply which will be operated by small dry battery.

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4. Quantum Mechanical Calculation on the Bond Moment.

Pauling's Formula about Electronegativity.

Nishio Hirai.

The bond moments of diatomic (F. T. Wall: J. A. C. S. **61**, 1051 (1939)) and polyatomic (T. Ri and N. Muroyama: Proc. Imp. Acad., **20**, 93 (1944); Rev. Phys. Chem. Japan, **18**, 24 (1944)) molecules were calculated by the resonance theory and given as follow,

$$\mu_{AB}=i^2 e r_{AB}, \quad 1/i^2=1+(E^0_{AB}-E_i)/E' \tag{1}$$

Here we will make clear the relation between μ and the difference in electronegativity of two atoms. When the bound is completely homopolar, its energy and Hamiltonian are

$$E^0_{AB}=\frac{1}{2}(E_{AA}+B_{BB}), \quad H^0_{AB}=\frac{1}{2}(H_{AA}+H_{BB}) \tag{2}$$

The difference in the effective nuclear charges is $\triangle Z$ and its effect can be considered as a perturbation to the complete homopolar bond, then

$$H_{AB}=H^0_{AB}+H', \quad H'=\frac{\triangle Z^2e^2}{2r_{AB}}-\frac{\triangle Ze^2}{2r_{AB}}\left(\frac{1}{r_{A2}}-\frac{1}{r_{B1}}\right) \tag{3}$$

can be derived from (2), and corresponding to this perturbation

$$\psi_{AB}=\psi^0_{AB}+\psi', \quad E_{AB}=E^0_{AB}+E', \quad \psi'=iA(1)\ A(2) \tag{4}$$

If we put $W_A=Z_Ae^2/2r_A \sim 110x_A$ for the atoms $r_{AB}\simeq r_A+r_B \doteqdot 2A$, the additional ionic resonance energy

$$E'=\iint \psi^0_{AB}H'\psi^0_{AB}d\tau_1 d\tau_2 \simeq \frac{\triangle Z^2e^2}{r_{AB}}=23\,(x_A-x_B)^2 \tag{5}$$

As for the amount of ionic charactor

$$i^2=H'^2_{0i}/(E^0_{AB}-E_i)^2=\triangle Z^2e^4J^2/2(E^0_{AB}-E_i)^2=\frac{1}{4}(x_A-x_B)^2 \tag{6}$$

If we put $J=\int A(1)\ B(1)\frac{1}{r_{A1}}d\tau_1 \doteqdot L/r_{AB}$ where we assume L is 0.65, the value of hydrogen-like wave function $1S$ and $2S$ at about $r_{AB}\doteqdot 2A$, and $E^0_{AB}-E_i\cong 90$ Kcal/mol (7) when $\triangle Z$ is small.

We can get (6) as the first term of Taylor expantion of (1) in x_A-x_B from (5) and (7).

Equation (5) and (6) are the empirical formulas which are given by L. Pauling in "The Nature of the Chemical Bond." 60, 69 (1940).